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Two regimes for effects of surface disorder on the zero-bias conductance peak of tunnel junctions involving d-wave superconductors

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Impurity-induced quasiparticle bound states on a pair-breaking surface of a d-wave superconductor are theoretically described, taking into account hybridization of impurity- and surface-induced Andreev states. Further a theory for effects of surface disorder (of thin impurity surface layer) on the low-bias conductance of tunnel junctions is developed. We find a threshold n_c for surface impurity concentration n_S, which separates the two regimes for surface impurity effects on the zero-bias conductance peak (ZBCP). Below the threshold, surface impurities do not broaden the ZBCP, but effectively reduce its weight and generate impurity bands. For low n_S impurity bands can be, in principle, resolved experimentally, being centered at energies of bound states induced by an isolated impurity on the surface. For larger n_S impurity bands are distorted, move to lower energies and, beginning with the threshold concentration $n_S = n_c$, become centered at zero energy. With increasing n_S above the threshold, the ZBCP is quickly destroyed in the case of strong scatterers, while it is gradually suppressed and broaden in the presence of weak impurity potentials. More realistic cases, taking into account additional broadening, not related to the surface disorder, are also considered.

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Inhomogeneities in anisotropically paired superfluids and superconductors can noticeably modify properties of adjacent regions on the scale of the coherence length. In particular, quasiparticle Andreev bound states can arise in those regions near impurities, surfaces or interfaces. Zero-energy Andreev bound states near impenetrable smooth surfaces of d-wave superconductors are known to be the signature of a sign change of the order parameter in a quasiparticle reflection event. In high-temperature superconductors the zero-energy states are identified, in particular, as resulting at low temperatures in the zero-bias conductance peak (ZBCP) of NIS-junctions (see, for example, review articles[1,2] and references therein).

In the present paper we report a theory for effects of surface disorder on the ZBCP and, more generally, the subgap conductance. Our starting point is the problem of quasiparticle bound states induced by an isolated impurity, situated close or directly on (110) surface of a d-wave superconductor. Spectra of the bound states can be found from the equation for the poles of the t-matrix, which takes the form

$$\det\left(\hat{1} - V_{imp}\hat{\tau}_3\hat{G}_0(\boldsymbol{r}_{imp}, \boldsymbol{r}_{imp}; \varepsilon)\right) = 0 \ . \qquad (1)$$

Here $\boldsymbol{r}_{imp}$ is the impurity position and V_{imp} the weight of the potential $V(\boldsymbol{r}) = V_{imp}\delta(\boldsymbol{r} - \boldsymbol{r}_{imp})$. For simplicity, we disregard here the effect of the impurity on the order parameter. The Nambu matrix retarded Green's function $\hat{G}_0(\boldsymbol{r}, \boldsymbol{r}'; \varepsilon)$ describes the system in the absence of the impurity. The quantity $\hat{G}_0(\boldsymbol{r}_{imp}, \boldsymbol{r}_{imp}; \varepsilon)$ with identical first and second coordinates is directly associated with the quasiclassical Green's function averaged over the Fermi surface: $\hat{G}_0(\boldsymbol{r}_{imp}, \boldsymbol{r}_{imp}; \varepsilon) = N_f \left\langle \hat{\tau}_3 \hat{g}_0(\boldsymbol{p}_f, \boldsymbol{r}_{imp}; \varepsilon)\right\rangle_{S_f}$. Here we omitted the term, which should be eventually included into the renormalized chemical potential; N_f is the normal state density of states on the Fermi surface per one spin direction, $\hat{\tau}_3$ is the respective Pauli matrix in particle-hole space. In the presence of (110) or (100) surfaces in a d-wave superconductor, the averaged off-diagonal components of the Green's function vanish $\left\langle f_0(\boldsymbol{p}_f, x; \varepsilon)\right\rangle_{S_f} = \left\langle f_0^+(\boldsymbol{p}_f, x; \varepsilon)\right\rangle_{S_f} = 0$ throughout the superconductor and for any ε. In this case we obtain the following equation for the spectrum of impurity bound states:

$$u\left\langle g_0(\boldsymbol{p}_f, \boldsymbol{r}_{imp}; \varepsilon)\right\rangle_{S_f} = \pm\pi \ , \qquad (2)$$

where dimensionless impurity potential is introduced $u = \pi V_{imp} N_f$. Near (100) surface the quasiclassical Green's function of a $d_{x^2-y^2}$-wave superconductor does not depend on spatial coordinates and takes the same form as in the bulk: $g_0(\boldsymbol{p}_f, \boldsymbol{r}; \varepsilon) = -i\pi\varepsilon \Big/ \sqrt{\varepsilon^2 - |\Delta(\boldsymbol{p}_f)|^2}$. Averaging this expression over a cylindrical Fermi surface and substituting into Eq. (2) leads to well established results on energies of impurity bound states in d-wave superconductors[3,4]. Qualitatively, a well pronounced low-energy resonance forms in the case of sufficiently large strength of the impurity potential, for instance, close to the unitarity limit. No resonance is present in the case of weakly scattering impurity, when subgap impurity states lie mostly at higher energies, being strongly broaden.

We demonstrate below, that impurity states near (110) surface have quite different structure as compared with the (100) case, as an effect of a hybridization of impurity- and surface-induced Andreev states. In the presence of (110) surface the quasiclassical Green's function of a $d_{x^2-y^2}$-wave superconductor is spatially dependent and

has a pole at zero energy, associated with zero-energy surface Andreev bound states. For this reason the spectrum of impurity bound states becomes dependent on the distance of the impurity from the surface. Assume, for simplicity, that the impurity is situated quite close or directly on (110) surface, so that the zero-energy surface states have strong influence on the formation of the impurity states. In contrast with the (100) case, a well pronounced low-energy impurity resonance $\varepsilon_{imp} = \varepsilon'_{imp} + i\varepsilon''_{imp}$, $|\varepsilon''_{imp}| \ll |\varepsilon'_{imp}|$ takes place in this case only for weakly scattering impurity potential. At low energies the pole-like term dominates the Green's function and in the first approximation $\left\langle g_0(\boldsymbol{p}_f, x=0; \varepsilon)\right\rangle_{S_f} = \frac{r}{\varepsilon + i0}$, where $r = \pi\left\langle\left|\tilde{\Delta}(\boldsymbol{p}_f)\right|\right\rangle_{S_f}$ is the residue of the pole-like term averaged over the Fermi surface. The quantity $\left|\tilde{\Delta}(\boldsymbol{p}_f)\right|$ coincides with the modulus of the bulk order parameter, if one disregards the surface pair-breaking. In general, it is a normalized integral over the superconductor, containing a spatially dependent (self-consistent) order parameter[5,6]. Inserting the pole-like term into the equation for impurity bound states, we find the energy of the resonance for weakly scattering impurity potential ($u \ll 1$): $\varepsilon'_{imp} = \pm ur/\pi$. In order to find the decay rate, one should keep also the first low-energy term in the imaginary part of the Green's function, averaged over the Fermi surface. For nonzero low energies, narrow vicinities near the nodes of the order parameter dominate the averaging of the imaginary part. Assuming a cylindrical Fermi surface, we find $\left\langle g_0(\boldsymbol{p}_f, x=0; \varepsilon)\right\rangle_{S_f} \approx \frac{r}{\varepsilon + i0} - i\pi\frac{|\varepsilon|}{\Delta_1}$, where Δ_1 is the slope of the order parameter at the node, taken in the bulk: $\Delta_1 = |\Delta'(\varphi_{node})|$. With this low-energy expression for the averaged Green's function we obtain from Eq.(2) for $u \ll 1$:

$$\varepsilon_{imp} = \varepsilon'_{imp} + i\varepsilon''_{imp} = \pm ur/\pi - ir^2u^3/(\pi^2\Delta_1) \ . \quad (3)$$

Self-consistent calculations give for (110) surface orientation $r \approx \Delta_0$ with a good accuracy, where Δ_0 is the maximum value of the bulk order parameter $\Delta(\boldsymbol{p}_f) = \Delta_0 \sin 2\varphi$. Impurity-induced subgap states in d-wave superconductors have Andreev origin. An imaginary part of the energy ε''_{imp} is associated with an escape of the quasiparticle from the impurity into the bulk of the superconductor. This can take place due to impurity scattering, if for an acquired momentum direction the quasiparticle energy exceeds the modulus of the d-wave order parameter. For sufficiently small energy $|\varepsilon'_{imp}| \ll \Delta_0$ a quasiparticle can run away from the impurity only with momenta in a narrow vicinity of nodal directions of the order parameter. Then a well pronounced impurity-induced quasiparticle resonance arises. For a larger subgap energy of impurity-induced state, the escape can occur in a wider region of momentum directions and the resonance is more broaden. As seen from Eq.(3), the resonance is well defined for weakly scattering impurity potential $u \ll 1$. In the opposite case of large strength of impurity potential $u \gtrsim 1$, the impurity states formally approach $|\varepsilon'_{imp}| \sim \Delta_0$ and the resonance itself is ill defined, because $|\varepsilon'_{imp}| \sim |\varepsilon''_{imp}|$.

Similar to the impurity in the bulk of d-wave superconductor[4], the local density of states (LDOS) at the impurity site near (110) surface manifests the particle-hole asymmetry: for repulsive impurity potential a resonance peak in the LDOS at this site takes place only for $\omega < 0$, while for attractive potential at $\omega > 0$. This property is directly associated with vanishing anomalous Gor'kov Green's function, describing the d-wave superconductor with (110) surface in the absence of the impurity and taken at one and the same site $F_0(\boldsymbol{r}_{imp}, \boldsymbol{r}_{imp}, \varepsilon) = N_f \left\langle f_0(\boldsymbol{p}_f, \boldsymbol{r}_{imp}; \varepsilon)\right\rangle_{S_f} = 0$.

The resonance energy is a function on the distance x_{imp} between the impurity and the (110) surface. At sufficiently large distances $x_{imp} \gg \xi_0, u\xi_0$ and not necessarily for weak scatterers, we obtain $\varepsilon'_{imp} = \pm \dfrac{u\mathrm{v}_f^2}{2\pi\Delta_1 x_{imp}^2}$, $\varepsilon''_{imp} = -\dfrac{3u^3\mathrm{v}_f^4}{8\pi^2\Delta_1^3 x_{imp}^4}$. The weight of the corresponding peak in the LDOS at the impurity location diminishes $\propto x_{imp}^{-2}$ with increasing x_{imp}, similar to the weight of the zero-energy peak originated from the surface bound states.

It turns out that changes in the LDOS due to the impurity resonance, take place entirely at the expense of the zero-energy surface states. The presence of a single impurity near (110) surface induces four quasiparticle impurity states: two spin degenerated states with positive and two with negative energies. Their contribution to the integral DOS is 2, since each spin-polarized Andreev state with nonzero energy contribute one half to the integral DOS[7,8]. In its turn, the number of the zero-energy Andreev surface states in the presence of one impurity reduces exactly by two (by one per spin polarization), as compared with the case of no surface defects. Thus, the total number of the surface and the impurity quasiparticle states keeps constant. This is valid, actually, for any number of impurities at (or near) the surface. The resonance energy and decay rate depend also on surface-to-crystal orientation. The above consideration can be easily generalized, with minor modifications, to a wide range of the orientations. Only for surface orientations very close to (100), when the residue of the zero-energy pole-like term becomes negligible (due to a small fraction of trajectories where the zero-energy surface states take place), a small low-energy term $-\frac{2\varepsilon}{\Delta_0}\ln\left(\frac{4\Delta_0}{-i\varepsilon}\right)$ dominates the averaged Green's function. As a result, the spectrum of impurity bound states on (100) surface coincide with the case of impurity-induced states in the bulk of a $d_{x^2-y^2}$-wave superconductor.

Consider further the low-energy LDOS and the low-bias tunnel conductance for the d-wave superconductor with (110) surface in the presence of many impurities. Since the conductance is sensitive mostly to impurities in the vicinity of the surface, we introduce below a thin surface layer of strongly disordered normal metal, which differs from the adjacent only by its very short mean

free path l. We consider a clean d-wave superconductor in the half-space $x > d$. The surface layer with impurity concentration n_{imp} is placed at $0 < x < d$ between a smooth impenetrable specularly reflecting surface at $x = 0$ and a clean superconductor at $x > d$. There are no additional potential barriers at $x = d$, between the disordered layer and the superconductor. The thickness d is assumed much less than all other characteristic scales in the problem. The model is very similar to the thin dirty layer model (TDL)[9] except that it incorporates the self-consistent t-matrix approach, allowing for arbitrary strength of quasiparticle scattering by impurities, while the TDL considers only the Born scattering. The other difference is that real surface layer of normal metal with isotropic impurities is introduced here, while special anisotropic scatterers (Ovchinnikov impurities) are used in the models of surface roughness[9,10]. Our results, presented below, can be easily reformulated for the case of Ovchinnikov impurities as well.

The quasiclassical 2×2 particle-hole matrix retarded Green's function $\hat{g}(\boldsymbol{p}_f, x; \varepsilon) = \begin{pmatrix} g & f \\ f^+ & -g \end{pmatrix}$ describes quasiparticle excitations and obeys Eilenberger's equations. For thin disordered surface layer with the impurity self-energy $\hat{\sigma}_{imp}(x;\varepsilon) \approx \hat{\sigma}_{imp}(0;\varepsilon)$, the surface impurity concentration $n_S = n_{imp} d$ and the surface impurity self-energy $\hat{\zeta}(\varepsilon) = 2i\hat{\sigma}_{imp}(x = 0;\varepsilon)d$ enter the final results. Off-diagonal elements of $\hat{\zeta}(\varepsilon)$ and $\langle \hat{g}(\boldsymbol{p}_f, x; \varepsilon)\rangle_{S_f}$ vanish in the case of (110) surface, so that $\hat{\zeta}(\varepsilon) = \zeta(\varepsilon)\hat{\tau}_3$.

The shape of the zero-energy peak in the density of states depends, to a great extent, on the surface self-energy $\zeta(\varepsilon)$. The surface self-energy, in its turn, is controlled by the Green's function averaged over the Fermi surface. We admit isotropic scatterers with arbitrary strength of potentials. Introducing a dimensionless surface impurity concentration $\tilde{n}_S = 2n_S/(\pi\hbar \mathrm{v}_f N_f)$, the surface self-energy parametrizes as:

$$\zeta(\varepsilon) = \frac{i\mathrm{v}_f \tilde{n}_S}{\pi} \frac{\langle g(\boldsymbol{p}_f, 0; \varepsilon)\rangle_{S_f}}{\dfrac{1}{u^2} - \dfrac{1}{\pi^2}\langle g(\boldsymbol{p}_f, 0; \varepsilon)\rangle^2_{S_f}} . \qquad (4)$$

For the low-bias conductance only the Green's function on the surface at low energies is of importance. The analytical solution we found for the model gives for low energies

$$g(\boldsymbol{p}_f, x = 0; \varepsilon) = -i\pi \coth\left(\frac{\zeta(\varepsilon)}{\mathrm{v}_f|\cos\varphi|} - i\frac{\varepsilon}{|\tilde{\Delta}(\boldsymbol{p}_f)|}\right) . \qquad (5)$$

Eqs. (4), (5) were derived exploiting the self-consistent spatial profile of the order parameter. Our further goal is to solve them jointly in some important particular cases and describe analytically the respective LDOS as a function of the energy, the surface impurity concentration and the strength of impurity potential. Also we represent below our fully self-consistent numerical results for conductance spectra, based on quasiclassical equations and boundary conditions for Riccati amplitudes of the quasiclassical matrix Green's function[11,12].

It turns out that the impurity layer is unable to broaden zero-energy surface bound states, if surface impurity concentration is less than the characteristic threshold: $\zeta(0) = 0$ for $\tilde{n}_S < \tilde{n}_c = \langle|\cos\varphi|\rangle_{S_f}$. As we found analytically, the delta-peak at zero energy occurs in the LDOS for all surface impurity concentrations below the threshold $n_S < n_c$ (see, e.g., Eq. (7)). Although, the weight of the peak is quite sensitive to n_S (see below). For the simplest model of a quasi-two-dimensional superconductor with cylindrical Fermi surface $\tilde{n}_c = 2/\pi$. The value $\tilde{n}_c$ is determined by the symmetry of pairing and does not depend on the particular spatial profile of the order parameter and the form of its basis functions. The threshold concentration of surface impurities exactly coincides with the number $N_0(0)$ of the zero-energy bound states per unit area of (110) surface in the absence of the disordered surface layer: $N_0(0) = n_c = (\pi/2)N_f \mathrm{v}_f \tilde{n}_c$. The effect is associated with detaching the states from the zero-energy peak in forming impurity bands. To a certain extent, this bears an analogy to what is known for impurity broadening of Landau levels and lifting of their degeneracy in the two-dimensional electron gas in a strong magnetic field[13,14,15]. In the presence of the disordered layer the number of zero-energy surface states linearly depends on the surface impurity concentration $\tilde{n}_S$ and vanishes at the threshold: $N_0(\tilde{n}_S) = N_0(0)(\tilde{n}_c - \tilde{n}_S)/\tilde{n}_c$. The threshold concentration remains equal to the number of the zero-energy states on the clean surface also for arbitrary surface misorientation angle α, not only for $\alpha = 45°$. For cylindrical Fermi surface $n_c(\alpha) = N_f \mathrm{v}_f \sqrt{1 - |\cos 2\alpha|}$. It approaches its maximal value for $\alpha = 45°$.

The behavior of the LDOS qualitatively differs below and above the impurity concentration threshold. In the presence of the surface impurity layer impurity bound states transform into two impurity bands, one with positive and the other with negative energies. For low concentrations of the Born impurities the bands are situated at low energies and the LDOS for the impurity bands takes the form

$$\nu(\varepsilon) = \frac{2\nu_{max}}{W}\sqrt{(W/2)^2 - (\varepsilon - \varepsilon'_{imp})^2} . \qquad (6)$$

This expression is valid in the energy range, where the argument of the square root function is positive. The characteristic bandwidth $W \sim \Delta_0 u\sqrt{\tilde{n}_S}$ and the height of the LDOS in the center of the band $\nu_{max} \sim \sqrt{\tilde{n}_S}/u$ are introduced in Eq. (6). Numerical coefficients in expressions for W and ν depend only on $|\tilde{\Delta}(\boldsymbol{p}_f)|$. We omit here respective cumbersome analytical formulas. In a good agreement with self-consistent calculations, the center of the Born impurity band is nothing but the position of the impurity resonance on the (110) surface: $|\varepsilon'_{imp}| = u\langle|\tilde{\Delta}(\boldsymbol{p}_f)|\rangle_{S_f}$. As seen from these estimations, the impurity hump rises, becomes more narrow and goes towards the zero energy, when the potential strength de-

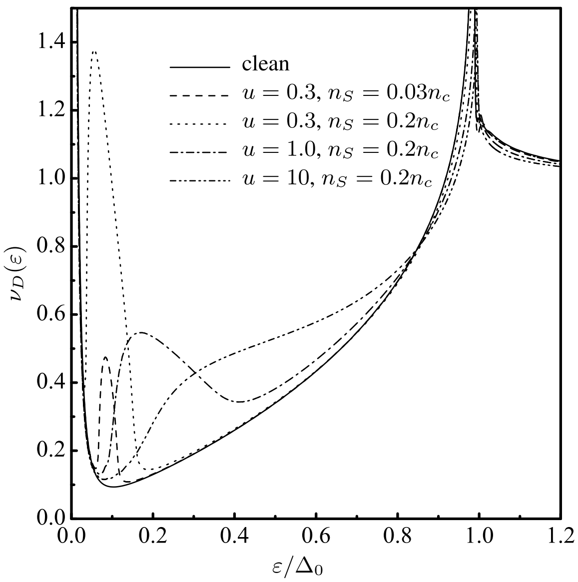

FIG. 1: Tunnel density of states on (110) surface as a function of energy. Solid line represents tunnel density of states for a smooth clean surface. Other curves describe effects of the surface impurity layer with various strengths of impurity potentials and surface impurity concentrations. Intrinsic broadening $0.002T_c$ is introduced for resolving the zero-energy δ-peak.

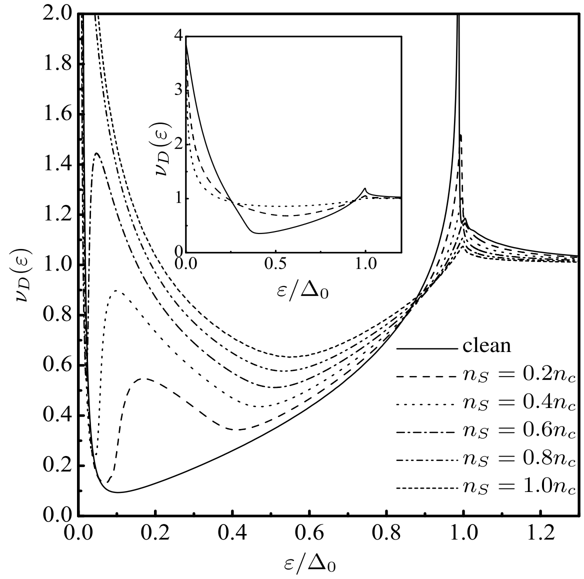

FIG. 2: Tunnel density of states on (110) surface as a function of energy, taken for various surface impurity concentrations below and at the threshold. The strength of the impurity potential is identical for all curves: $u = 1$. Inset shows the tunnel density of states for impurity concentrations above the threshold: solid line – $n_S = 2.5n_c$, $u = 0.3$, dashed line – $n_S = 1.2n_c$, $u = 1$, dotted line – $n_S = 1.07n_c$, $u = 10$.

creases. Eq. (6), describing the shape of the impurity band in the LDOS, is valid only for small surface impurity concentration $u\nu_{max} \sim \sqrt{\tilde{n}_S} \ll 1$ and implies that the width of the impurity band significantly exceeds the width of separate impurity resonance $W \gg |\varepsilon''_{imp}|$.

Fig. 1 displays the energy dependence of the tunnel density of states (i.e. the conductance at $T = 0$) for clean (110) surface, as well as for surface disordered layers with various strengths of impurity potentials. Here and below the momentum dependence of the transparency of NIS junction is taken in the simple form $D(\varphi) = D_0 \cos^2 \varphi$, suitable for thin and high potential barriers. Tunnel DOS and conductance are normalized to their normal state values. At those energies, where the impurity peak stands out well against the background, the tunnel density of states is simply proportional to the LDOS on the surface with the energy-independent coefficient of the order of unity. Eq.(6) describes with a good accuracy impurity peaks on two curves with $u = 0.3$ in Fig. 1. The impurity peaks are situated sufficiently close to the zero-energy peak. In the case $u = 0.3$, $n_S = 0.2n_c$ the impurity peak has a small asymmetric distortion, which is not taken into account in Eq.(6). With increasing u the impurity bands become less pronounced, more asymmetric and broaden. For sufficiently large u impurity bands are strongly broaden at low n_S over all subgap region.

Fig. 2 shows the evolution of impurity bands with varying the surface impurity concentration below the threshold for the impurity potential $u = 1$. The impurity peak goes towards the lower energies and rises when the concentration increases. Beginning with the threshold concentration impurity bands are centered on zero energy, for any strength of impurity potential. At the threshold concentration an impurity-induced zero-energy peak in the tunnel DOS arises with a specific power-law spectral shape $\nu_D(\varepsilon) \propto |\varepsilon|^{-1/3}$ in the low-energy region $\ln(\Delta_0/|\varepsilon|) \gg 1$. This peak takes place for arbitrary strength of impurity potential.

The weights of the ZBCP and the zero-energy peak in the LDOS, associated with the surface zero-energy Andreev states, reduce with increasing n_S. Below the threshold they vary linear in $(\tilde{n}_c - \tilde{n}_S)$, within the logarithmic accuracy, and vanish at $n_S = n_c$. Close to the threshold $0 < \tilde{n}_c - \tilde{n}_S \ll \tilde{n}_c$ the low-energy momentum resolved LDOS

$$\nu(\varphi, x = 0; \varepsilon) = \frac{\pi|\cos\varphi|\,(\tilde{n}_c - \tilde{n}_S)}{\mathcal{S}_0 \ln\left[\dfrac{\tilde{\mathcal{S}}\mathcal{S}_0\tilde{\Delta}_{max}}{\tilde{n}_c - \tilde{n}_S}\right]}\,\delta(\varepsilon). \tag{7}$$

Here $\mathcal{S}(x) = \left\langle \cos^2\varphi\, \delta(x - |\tilde{\Delta}(\boldsymbol{p}_f)|)\right\rangle_{S_f}$, $\mathcal{S}_0 = \mathcal{S}(x \to +0)$, $\mathcal{S}_0 \ln\tilde{\mathcal{S}} = \int_0^\infty \mathcal{S}'(x)\ln(\tilde{\Delta}_{max}/x)dx$ and $\tilde{\Delta}_{max}$ is a maximal value of $|\tilde{\Delta}(\boldsymbol{p}_f)|$ over Fermi surface. For cylindrical Fermi surface $\mathcal{S}_0 = 2/\pi\Delta_1$. With spatially constant order parameter we also find $\tilde{\mathcal{S}} = 2$. Eq. (7) is valid for low energies $|\varepsilon| \ll (\tilde{n}_c - \tilde{n}_S)\Delta_1$, $(\tilde{n}_c - \tilde{n}_S)^{3/2}u\Delta_1$, where one can disregard the contribution from impurity bands.

Above the threshold $\tilde{n}_S > \tilde{n}_c$ the solution of Eqs.(4), (5) results in the following angular resolved surface density of states at zero energy

$$\nu(\varphi, 0; 0) = \frac{\left(\dfrac{3\pi^2}{2u^2} + \ln\left[\dfrac{13.1}{\tilde{n}_S - \tilde{n}_c}\right]\right)^{1/2}}{\sqrt{6(\tilde{n}_S - \tilde{n}_c)}} |\cos\varphi| \ . \qquad (8)$$

This finite zero-energy value of the density of states, together with the low-energy corrections (see, e.g., Eq.(9)), describes the broaden zero-energy peak above the threshold. The condition $\zeta(0)/\mathrm{v}_f \ll 1$ implied in the derivation of Eqs.(8) applies not only close to the threshold. For sufficiently weak scatterers, when the large term $3\pi^2/2u^2$ dominates the logarithmic function, the expression for $\zeta(0)/\mathrm{v}_f$ remains also small for $\tilde{n}_S \gg \tilde{n}_c$. The Born approximation works in this case and we find $\nu(\varphi, x = 0; \varepsilon = 0) = |\cos\varphi|/(\rho\tilde{n}_c)^{1/2}$, where $\rho = u^2\tilde{n}_S = d/l$. Here $l = \mathrm{v}_f\tau$ and τ are the mean free path and the relaxation time in the disordered layer. The inset of Fig. 2 demonstrates the behavior of the low-energy tunnel density of states above the threshold. The heights of ZBCP, which can be obtained from Eq. (8), are in agreement with those in the inset of Fig. 2 within few percents.

Usually, the Born approximation is justified, if the first term in the denominator of Eq.(4) dominates the second one, i.e. the relation $u^2|\left\langle g(\boldsymbol{p}_f, 0; \varepsilon)\right\rangle^2_{S_f}|/\pi^2 \ll 1$ satisfies. The unitary approximation works in the opposite limit. In ordinary normal metals $|\left\langle g(\boldsymbol{p}_f, 0; \varepsilon)\right\rangle^2_{S_f}|/\pi^2 = 1$ and the condition for the Born (unitary) approximation to be valid reduces to the standard form: $u^2 \ll 1$ ($u^2 \gg 1$). In superconductors the quantity $|\left\langle g(\boldsymbol{p}_f, 0; \varepsilon)\right\rangle^2_{S_f}|/\pi^2$ can strongly deviate from unity at low energies. In the absence of zero-energy (low-energy) states we have at low energies $|\left\langle g(\boldsymbol{p}_f, 0; \varepsilon)\right\rangle^2_{S_f}|/\pi^2 \ll 1$. This expands the region of applicability of the Born approximation in superconductors at low energies. However, in the presence of the zero-energy surface bound states the pole-like term dominates the Green's function and takes very large values on the surface at low energies. Moreover, since the zero-energy states are dispersionless states, the Green's function, taken on the boundary at low energies, remains to be quite large even after averaging over the Fermi surface. Then, at sufficiently low energies we obtain $|\left\langle g(\boldsymbol{p}_f, 0; \varepsilon)\right\rangle^2_{S_f}|/\pi^2 \gg 1$. This condition strongly modifies the behavior of the results, obtained in the Born and in the unitary approximations[16]. It is also seen, that even though there are Born impurities in the disordered surface layer on the normal metal sample ($u^2 \ll 1$), in the case of the superconducting substrate the presence of zero-energy surface states places additional restrictions on admitting the Born approximation to the same scatterers. They can scatter low-energy quasiparticles near the surface with a large effective strength. This takes place, if the impurity concentration is not sufficiently high and the zero-energy peak in the LDOS is well pronounced.[17] Under certain conditions the weak impurity potentials $u^2 \ll 1$ can be described even with unitary approximation in the presence of the zero-energy surface states. This applies below the threshold to describing the zero-energy peak and turns out to be very important for our results. This is very different from various other circumstances where the Green's function doesn't take large values and the Born approximation can always be justified for sufficiently weak scatterers.

We find, that the Born approximation applies for describing sufficiently high zero-energy peaks in the density of states, only if the surface impurity concentration well exceeds the threshold surface concentration: $n_S \gg n_c$.[18] This condition can be quite restrictive. A simple estimation gives $n_c \sim \hbar\mathrm{v}_f N_f \sim a n_e$, a being the interatomic distance and n_e the electron concentration. For optimally doped $YBa_2Cu_3O_{7-\delta}$ cut with (110) surface, we evaluate the threshold surface concentration as $n_c \approx 1.3 \times 10^{14}\mathrm{cm}^{-2}$. This is sufficiently large (although well accessible) value of the threshold for the surface concentration of point defects.

Conditions for the applicability of the Born and the unitary approximations modify further for surface impurity concentrations close to the threshold. The self-consistent analysis of Eqs. (4), (5) shows that at $n_S \approx n_c$ the two large terms, which usually dominate the low energy behavior of $\left\langle g(\boldsymbol{p}_f, 0; \varepsilon)\right\rangle_{S_f}$, almost cancel each other. Then conventional criteria for the Born ($u \ll 1$) and the unitary ($u \gg 1$) approximations recover with a logarithmic accuracy. In particular, this kind of conditions for the Born or the unitary approximations arises in Eq.(8), depending on what term in the numerator dominates.

A characteristic feature of the zero-energy peak in the LDOS above the surface concentration threshold, is a cusp-like shape of the peak. Indeed, the first low-energy correction to the LDOS turns out to have a characteristic energy dependence $\left\langle\delta\nu(\varphi, x = 0; \varepsilon)\right\rangle_{S_f} \equiv \left\langle\nu(\varphi, 0, \varepsilon) - \nu(\varphi, 0, 0)\right\rangle_{S_f} \propto |\varepsilon|$. The cusp-like shape of the broaden zero-energy peak is clearly seen on the inset of Fig. 2 (see also Fig. (6c) in Ref. 19, obtained with the thin dirty layer model and Ovchinnikov impurities). While the zero-energy peak in the LDOS originates from the sign change of the order parameter in a quasiparticle reflection from the surface, the cusp-like behavior of the peak comes from the narrow vicinities of the order parameter nodes. Since for (110) surface only the momentum directions close to the surface normal are of importance, the tunnel DOS at low energies acquires the same cusp-like behavior $\sim |\varepsilon|$, although with a different numerical coefficient. In the unitary limit, when the zero-energy density of states is described by Eq.(8) with $u \gg 1$, we get

$$\left\langle\delta\nu(\varphi, 0; \varepsilon)\right\rangle_{S_f} = -\frac{\pi^2|\varepsilon|\mathcal{S}_0}{8}\frac{\nu^4(0)}{\nu^2(0)(\tilde{n}_S - \tilde{n}_c) - 4/(3\pi^3)}. \qquad (9)$$

This term becomes comparable with $\left\langle\nu(\varphi, x = 0; 0)\right\rangle_{S_f} = \nu(0)$ for $\varepsilon \sim (\tilde{n}_S - \tilde{n}_c)^{3/2}$. Our estimations for sufficiently high and narrow ZBCP show that the width of the

peak manifests analogous dependence $\gamma \sim (\tilde{n}_S - \tilde{n}_c)^{3/2}$.

In the Born limit we obtain $\langle \delta\nu(\varphi, x=0;\varepsilon)\rangle_{S_f} \approx -\pi|\varepsilon|/(4\rho\Delta_1)$. This quantity is of the order of the zero-energy surface density of states $\sim 1/(\rho\tilde{n}_c)^{1/2}$ for $\varepsilon \sim \gamma \propto \rho^{1/2}$. For the Born surface disordered layer $\zeta(0)/\mathrm{v}_f = \sqrt{\rho\tilde{n}_c}$. It follows from here $\gamma \propto \sqrt{\rho} \propto \tau^{-1/2}$. We note, that the relation $\gamma \propto \tau^{-1/2}$ is a common feature of the broadening of the zero-energy surface bound states by Born scatterers, doesn't matter whether they are spread out as bulk impurities[16], occupy a surface layer with the thickness of the order or larger than the coherence length[20], or are collected only in a very thin surface layer as it is the case in the present paper. The width of a well pronounced impurity band turns out to be $\propto \sqrt{n_{imp}}$ also below the threshold, as it is for W in Eq.(6), as well as in some other circumstances[21,22].

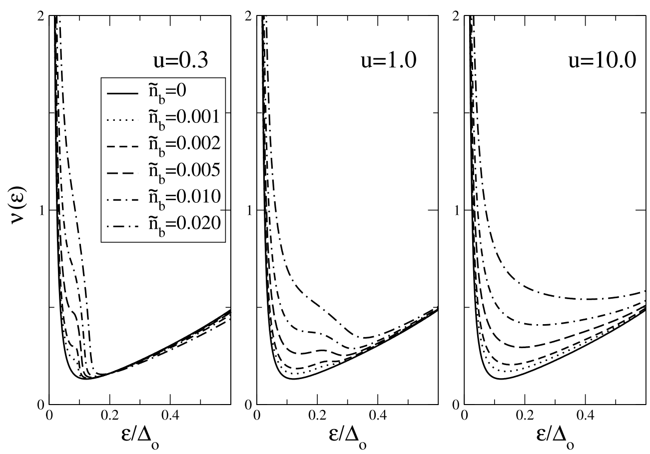

FIG. 3: LDOS on (110) surface as a function of energy, taken for three values of strength of impurity potential u and for various bulk impurity concentrations. Dimensionless concentration of bulk impurities $\tilde{n}_b$ is defined as $n_b = 2\pi^2 N_f T_c \tilde{n}_b$. The lower curve corresponds to clean superconductor $\tilde{n}_b = 0$. With $\tilde{n}_b = 0$; 0.001; 0.002; 0.005; 0.01; 0.02 one goes from the lower to the upper curve on each panel. Impurity humps are present for $u = 0.3$, $u = 1.0$ for a certain range of concentrations n_b.

Consider further more realistic cases, taking into account also some other reasons, not related to the surface disorder, which can result in a broadening of the ZBCP in both regimes studied above. Let, for example, impurities occupy not only the surface layer with surface impurity concentration n_S, but also are spread out over an extensive region of a superconductor as bulk impurities with small bulk concentration n_b. Since energies of surface impurity states depend on distance x_{imp}, in the presence of bulk impurities it is not obvious whether impurity bands are fully smeared out and merge in a periphery of the zero-energy peak, or they still survive, being centered at energies of surface impurity states Eq.(3) for low n_S. For making clear this question we have studied, firstly, the effect of bulk impurities only. Fig. 3 shows the LDOS

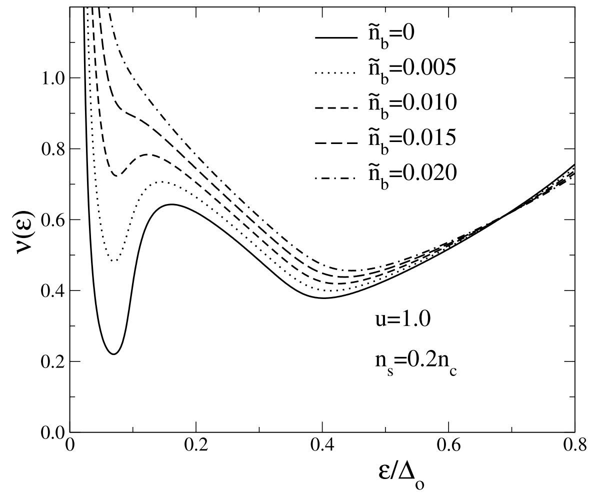

FIG. 4: LDOS on (110) surface in the presence of bulk and surface impurities, taken for various bulk impurity concentrations $\tilde{n}_b$, as a function of energy. The strength of impurity potential $u = 1$, the surface impurity concentration $n_S = 0.2n_c$.

on (110) surface for a superconducting d-wave half-space with small bulk impurity concentration n_b, which is constant everywhere up to (110) surface. As seen, surface impurity bands survive in the LDOS for weak scatterers ($u = 0.3$ and $u = 1$) in a range of bulk impurity concentrations n_b. Although, the bands are less pronounced and take place in a more narrow region of n_b, as compared with Figs. 1, 2 for the surface impurity layer model. With increasing potential strength or/and impurity concentration n_b, impurity bands are gradually smeared out and merge in the zero-energy peak.

Effects of bulk impurities in the presence of thin surface impurity layer on the LDOS on (110) surface, are shown in Fig. 4 for $n_S = 0.2n_c$ and various n_b. Dimensionless concentration of bulk impurities is defined as $n_b = 2\pi^2 N_f T_c \tilde{n}_b$. One can see, that bulk impurities control the broadening of the zero-energy peak, when surface disorder lies well below the threshold. The zero-energy peak and the impurity bands fully merge into one broaden peak for comparatively small concentration of bulk impurities $n_b \approx 0.04\pi^2 N_f T_c$. Even in this case the height of the zero-energy peak is sensitive to the surface disorder, which controls relative weights of central and peripheral regions of the broaden zero-energy peak. The "fine structure" of the peak can be resolved only for less n_b. Then well above the threshold concentration the surface layer controls the broadening. Fig. 5 shows the evolution of the low-energy LDOS with the surface impurity concentration n_S in the surface layer, in the presence of bulk impurities ($n_b = 0.05\pi N_f T_c$). The inset of Fig. 5 shows the broadening γ of the zero-energy peak as a function of surface impurity concentration n_S/n_c, taken for various bulk impurity concentrations $\tilde{n}_b$. The broadening γ is the half of the width of the zero-energy peak: $\nu(0) = 2\nu(\gamma)$. As seen in the inset of Fig. 5, already at small concentrations bulk impurities transform

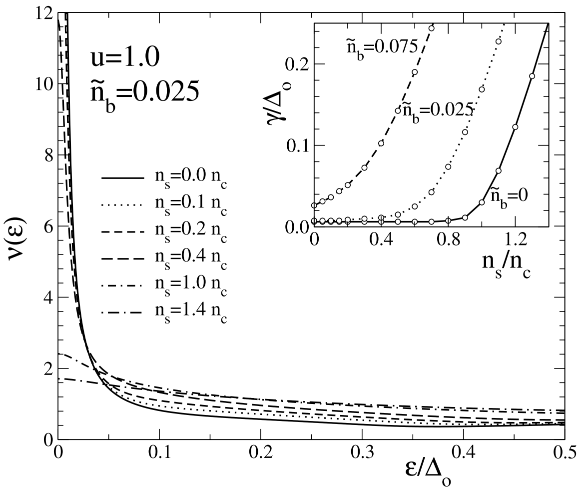

FIG. 5: LDOS on (110) surface in the presence of bulk and surface impurities, taken for various surface impurity concentrations n_S. The strength of impurity potential $u = 1$, the bulk impurity concentration $\tilde{n}_b = 0.025$. Inset shows the broadening γ of the zero-energy peak as a function of surface impurity concentration n_S/n_c, taken for various bulk impurity concentrations $\tilde{n}_b$.

an abrupt change of the regimes of the broadening at the threshold into a gradual crossover from one regime to another.

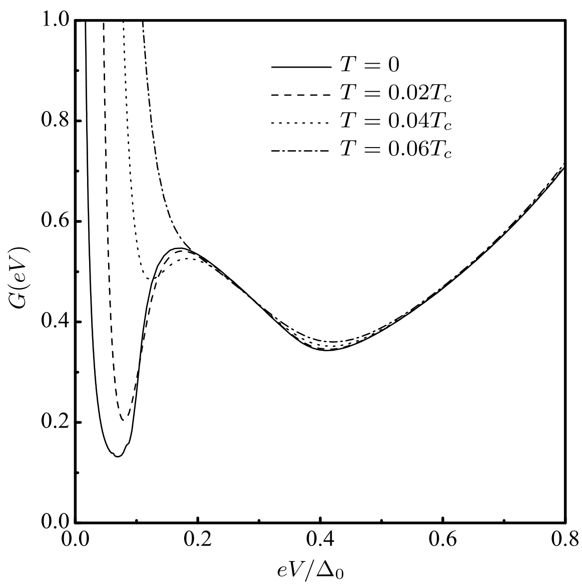

FIG. 6: Tunnel conductance on (110) surface for various temperatures as a function of the applied voltage. With increasing the temperature the ZBCP and impurity states broaden and strongly overlap. The strength of impurity potential and the concentration are identical for all curves: $u = 1$, $n_S = 0.2n_c$.

Effects of finite temperatures also contribute to a

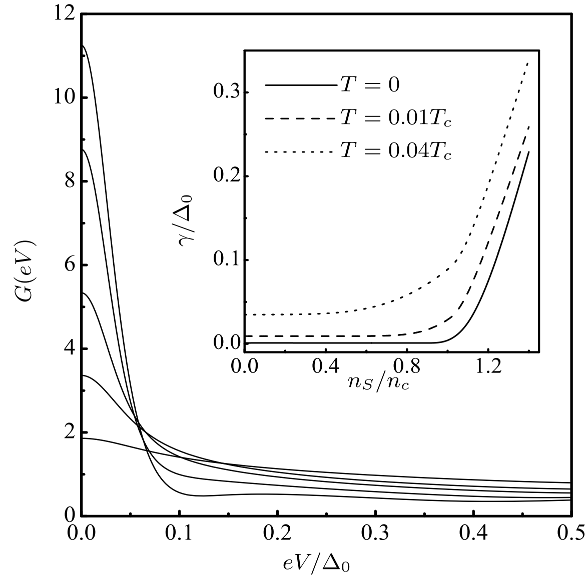

FIG. 7: Tunnel conductance on (110) oriented surface as a function of applied voltage for different impurity concentration $n_S = 0.2n_c$, $n_S = 0.4n_c$, $n_S = 0.7n_c$, $n_S = 1.0n_c$, $n_S = 1.4n_c$. Higher ZBCP corresponds to lower concentration. Temperature and scattering impurity potential are the same for all curves: $T = 0.04T_c$, $u = 1$. Inset shows the broadening γ of the ZBCP as a function of surface impurity concentration, taken for various temperatures: solid line – $T = 0$, dashed line – $T = 0.01T_c$, dotted line – $T = 0.04T_c$.

broadening and a suppression of the ZBCP, does not matter in the presence or absence of surface disorder. The tunnel conductance as a function of the applied voltage is shown on Fig. 6 for various temperatures. The temperature broadening of both the zero-energy and the impurity peaks takes place. The peaks fully merge into the one broaden peak above a comparatively low temperature, which is $\approx 0.06T_c$ for the particular case, considered on Fig. 6. The "fine structure" of the ZBCP arises below this temperature. In the cases we consider, impurity bands result in two humps (small satellites) whose heights are usually noticeably less than the ZBCP in the self-consistent calculations. Only for concentrations very close to the threshold the impurity peaks can become high and centered very close to zero energy, while the zero-energy peak is already exhausted. We tried to single out, whether this kind of "spontaneous splitting" of one broaden ZBCP into two separate low-energy peaks can be observed below a characteristic temperature in the case of high spectral resolution. Within the self-consistent t-matrix approximation and for all sets of parameters we used, three peaks always merge into one broaden peak before a "spontaneous splitting" described above could show up.

Fig. 7 shows the temperature broadening of the ZBCP for various surface impurity concentrations. As seen in the range of low n_S, the broadening of the ZBCP, being

fixed by the temperature, is almost insensitive to n_S. At the same time the height of the peak noticeably decreases with increasing n_S. The inset of Fig. 7 demonstrates that effects of finite temperatures, analogously to the effect of bulk impurities, transform the abrupt change of the regimes at the threshold into a gradual crossover from one regime to another. The surface impurity concentration can strongly influence the width of the ZBCP only above the crossover region, while the height of the ZBCP can be sensitive to the surface disorder for any n_S.

Results of the present paper apply to tunnel junctions, when the quasiparticle escape from the superconductor to the normal metal does not have strong influence on the broadening of the zero-energy states[6,23]. For higher transparencies this mechanism of the broadening becomes important. An information to what extent impurities and effects of finite transparency are involved into forming the broadening of the ZBCP in a particular NIS junction, in principle, could be obtained experimentally, e. g. by measurements of the differential shot noise at low voltages[24].

Thus, in the case of strong broadening of the ZBCP, induced by sources, which are not related to the surface disorder, impurity bands and the zero-energy peak, associated with Andreev surface states, merge into one broaden ZBCP. This can be associated also with the experimental resolution of the spectral weight. Even in this case the height of the ZBCP is quite sensitive to the surface disorder, whereas the width is not, since the disorder controls relative weights of central and peripheral regions of the broaden ZBCP. For a weak broadening and high experimental resolution impurity bands can be identified, at least for low n_S and u, as low-energy humps near the zero-energy peak. When n_s goes up, the bands become more close to the zero energy. Then more resolution and less broadening are needed for identifying them as separated from the zero-energy peak. For concentrations $n_S \geq n_c$ impurity bands with positive and negative energies merge into one impurity band, centered at zero energy. Sources, not related to the surface disorder, transform an abrupt change of the regimes of broadening of the ZBCP, into a gradual crossover from one regime to another. While the height of the ZBCP can be dominated by the surface disorder for any n_S, its width is always independent of n_S below the crossover region. Above the crossover the surface disorder can strongly influence the broadening of the ZBCP. It is worth noting, that special experimental study of effects of surface disorder on the shape of the ZBCP has been carried out in Ref. 25, where various degrees of the surface quality have been prepared by changing ion irradiation of $YBa_2Cu_3O_{7-\delta}$/Pb junctions. It was found in a certain range of irradiation doses, that the ZBCP width is almost unchanged as a function of surface disorder, while the height of the peak effectively decreases with increasing the irradiation effects. This kind of behavior is in agreement with theoretical results of the present paper.

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[18] Analogous condition can be obtained for scatterers, which are homogeneously spread out as bulk impurities in a d-wave superconductor up to (110) smooth surface, assuming that the zero-energy peak in the LDOS is sufficiently high. In terms of results of Ref. 16 we find in this case, that the condition for the Born approximation to apply to low-energy quasiparticle scattering by impurities near the surface takes the form $n \gg N_f \Delta_0$.

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